

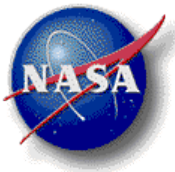
Anaconda on ADAPT (Brown Bag)

NCCS

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The Anaconda logo is a blue speech bubble shape with a small tail pointing downwards. The word "Anaconda" is written in white, sans-serif font inside the bubble.

Anaconda

Anaconda is a package management system that allows users to create independent environments each with different configurations of packages within them.

The Anaconda logo is a blue speech bubble shape with a small tail pointing downwards. The word "Anaconda" is written in white, sans-serif font inside the bubble.

Anaconda

Good News!

Users do NOT need to install Anaconda in personal directories!

Anaconda is already installed globally and can be imported/loaded across ADAPT VMs.

Agenda



Anaconda location



Anaconda Modules
(Finding and loading)



Anaconda Environments
(what envs?, Activating)



Creating a conda env
(customize and configure)



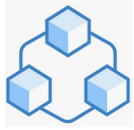
Anaconda location

Which Anaconda are you pointing to?

sstrong@foyer101:~\$ which conda

/att/opt/other/centos/anaconda3/bin/conda

*note-If no path is returned then an anaconda module will need to be loaded (discussed in module section)



Anaconda Modules



What is a
Module



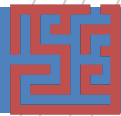
Enable “Module”
commands



Finding available
Modules



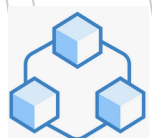
Loading available
Modules



What is a Module

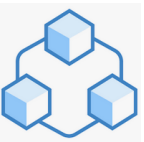
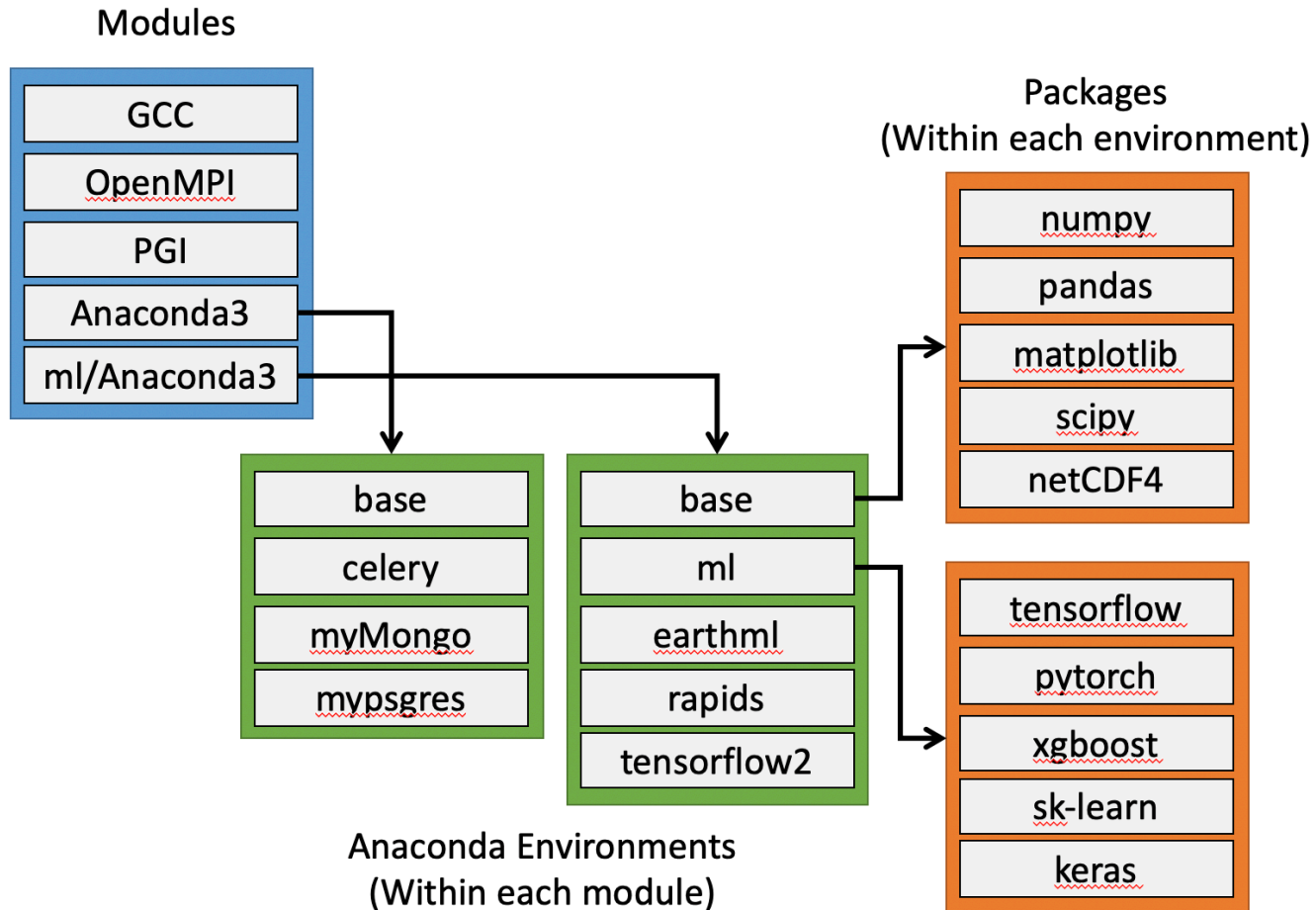
Modules are globally installed applications that ADAPT makes accessible to users across any VM on ADAPT.

Implemented by system admins, they contain commands that load specific applications into a users environment





What is a Module





Enable "module" commands

```
sstrong@foyer101:~$ echo $0  
-bash
```

```
sstrong@foyer101:~$ source  
/att/opt/other/centos/modules/init/bash
```

```
sstrong@foyer101:~$ export  
MODULEPATH=/att/opt/other/centos/modules/modulefiles
```

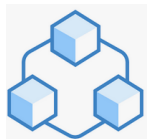




Finding Available Modules

```
sstrong@foyer101:~$ module av  
----- /att/opt/other/centos/modules/modulefiles -----  
anaconda3                jessie/R-3.6.1          ml/openmpi-4.0-gcc-9.1  
anaconda3_stratus        lmod/lmod_8.1           ml/PGI-18.10-OpenMPI-CUDA  
cmake-3.15.4              lmod/lua_5.1            module-info  
crane/R-3.6.1             lmod/tcl_8.9            openmpi-4-gcc-9.1-foyer  
gcc-7.4-explore           ml/anaconda3            openmpi-4.0.0-gcc-9.1  
gcc-9.1                   ml/bison-3.4            redis  
gcc-9.1-foyer             ml/CUDA-10.0            stretch/anaconda3  
gcc-9.1-ml4               ml/gcc-9.1              stretch/anaconda3_intern  
git-2.23.0                ml/hdf5-1.10.5-openmpi-4 stretch/bzip2  
hdf5-1.10.5-openmpi-gcc-9.1 ml/NCCL-2.3             stretch/jdk-13  
intel-19.0.2.187          ml/openmpi-4            stretch/R-3.6.1  
sstrong@foyer101:~$
```

**This a list of all the available system modules
(*note list is as of Dec 2019)**





Loading Available Modules

```
sstrong@foyer101:~$ module list
```

```
Currently Loaded Modulefiles:
```

```
1) anaconda3
```

```
sstrong@foyer101:~$ module av
```

```
----- /att/opt/other/centos/modules/modulefiles -----
```

anaconda3	jessie/R-3.6.1	ml/openmpi-4.0-gcc-9.1
anaconda3_stratus	lmod/lmod_8.1	ml/PGI-18.10-OpenMPI-CUDA
cmake-3.15.4	lmod/lua_5.1	module-info
crane/R-3.6.1	lmod/tcl_8.9	openmpi-4-gcc-9.1-foyer
gcc-7.4-explore	ml/anaconda3	openmpi-4.0.0-gcc-9.1
gcc-9.1	ml/bison-3.4	redis
gcc-9.1-foyer	ml/CUDA-10.0	stretch/anaconda3
gcc-9.1-ml4	ml/gcc-9.1	stretch/anaconda3_intern
git-2.23.0	ml/hdf5-1.10.5-openmpi-4	stretch/bzip2
hdf5-1.10.5-openmpi-gcc-9.1	ml/NCCL-2.3	stretch/jdk-13
intel-19.0.2.187	ml/openmpi-4	stretch/R-3.6.1

```
sstrong@foyer101:~$ module switch anaconda3 ml/anaconda3
```

```
sstrong@foyer101:~$ module list
```

```
Currently Loaded Modulefiles:
```

```
1) ml/anaconda3
```

```
sstrong@foyer101:~$ module switch ml/anaconda3 anaconda3
```

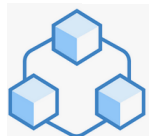
```
sstrong@foyer101:~$ module list
```

```
Currently Loaded Modulefiles:
```

```
1) anaconda3
```

```
sstrong@foyer101:~$ █
```

anaconda3 module loaded





Anaconda Environments



Conda envs
In Anaconda3



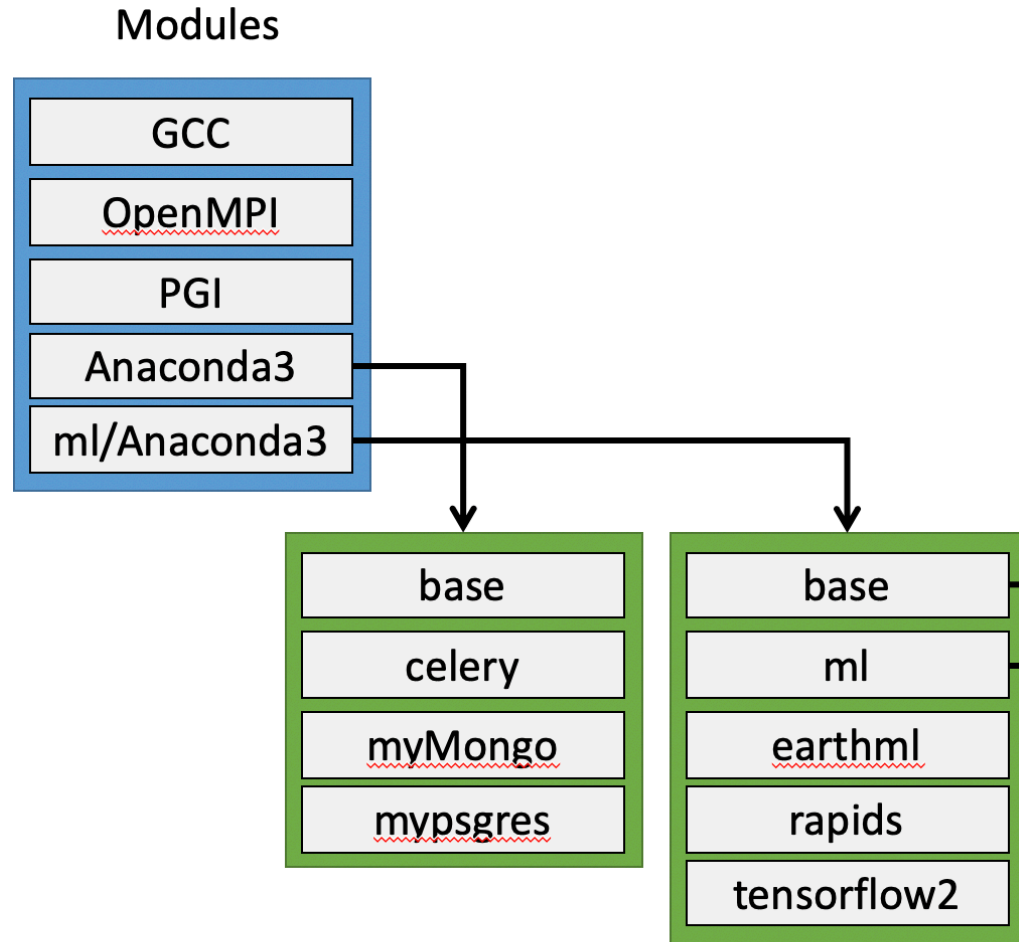
Find Packages
in a conda env



Activate and
deactivate a conda env



Conda Envs within base Anaconda3





```
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
                /att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest
                /att/nobackup/sstrong/conda/envs/edas-stratus
base             *  /att/opt/other/centos/anaconda3
celery           /att/opt/other/centos/anaconda3/envs/celery
earthml          /att/opt/other/centos/anaconda3/envs/earthml
myMongo          /att/opt/other/centos/anaconda3/envs/myMongo
mypsgres         /att/opt/other/centos/anaconda3/envs/mypsgres
r-environment    /att/opt/other/centos/anaconda3/envs/r-environment
baseclone        /home/sstrong/.conda/envs/baseclone

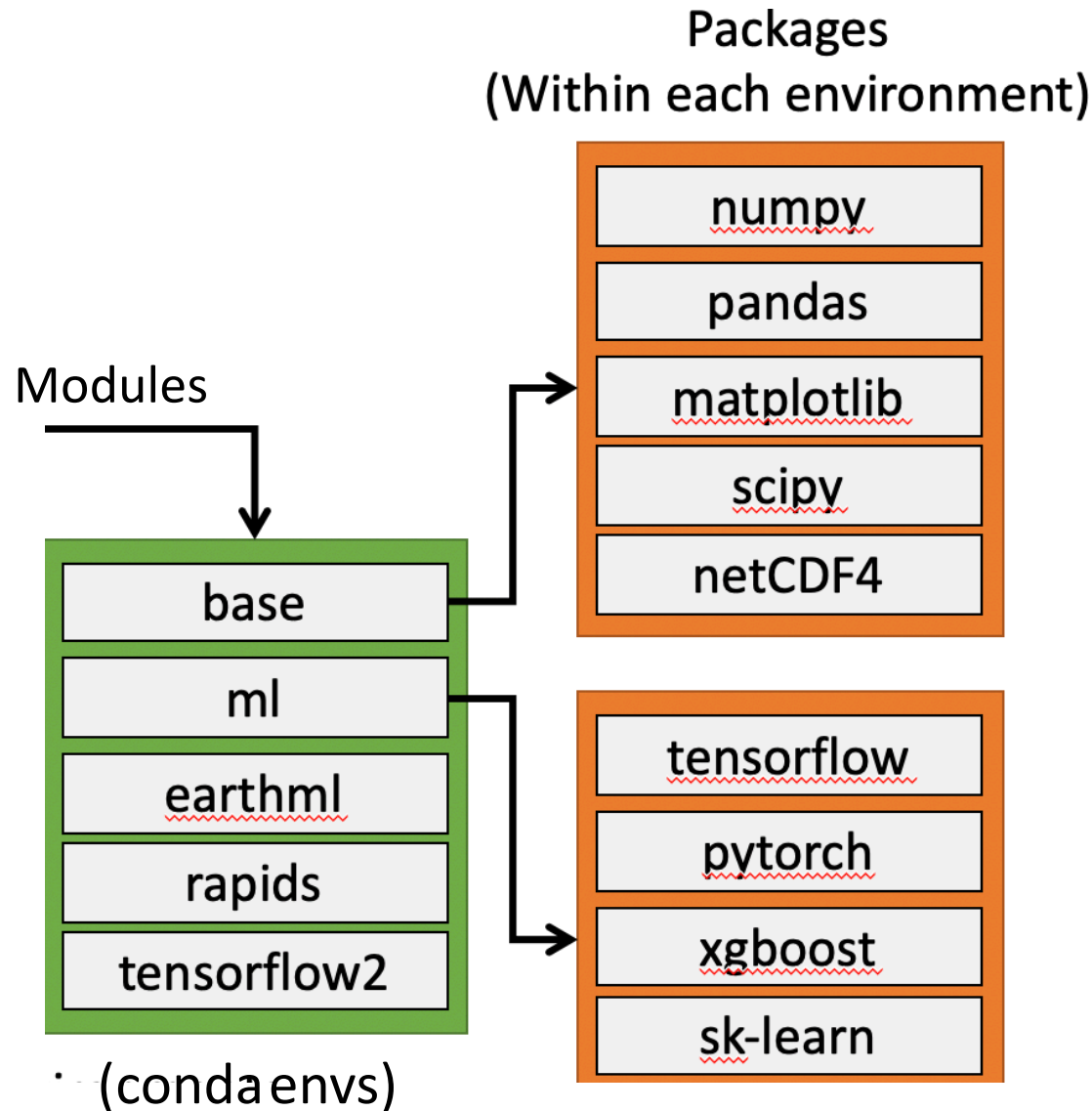
sstrong@foyer101:~$
```

"conda env list" will list all the environments within an anaconda module as well as all of the user's personally created environments.





Pkgs within a conda env





Find pkgs in a conda env

```
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/bin/conda
sstrong@foyer101:~$ conda list
# packages in environment at /att/opt/other/centos/anaconda3:
#
# Name                                Version                                Build      Channel
_ipyw_jlab_nb_ext_conf               0.1.0                                py37_0
_libgcc_mutex                         0.1                                  main
_r-mutex                             1.0.0                                anacondar_1
absl-py                              0.7.1                                py37_0     conda-forge
affine                               2.2.2                                py_0       conda-forge
alabaster                            0.7.12                               py_0       conda-forge
anaconda-client                      1.7.2                                py_0       conda-forge
anaconda-navigator                   1.9.6                                py37_0
asn1crypto                           0.24.0                               py37_1003  conda-forge
astor                                0.7.1                                py_0       conda-forge
astroid                              2.2.5                                py37_0     conda-forge
astropy                              3.2.1                                py37h516909a_0 conda-forge
attrs                                19.1.0                               py_0       conda-forge
babel                                2.7.0                                py_0       conda-forge
backcall                             0.1.0                                py_0       conda-forge
basemap                              1.2.0                                py37h673bf1a_1001 conda-forge
basemap-data-hires                   1.2.0                                0
beautifulsoup4                       4.7.1                                py37_1001  conda-forge
binutils_impl_linux-64               2.31.1                               h6176602_1
```

Packages within the basic anaconda3 env





Conda activate

```
|ssstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
|ssstrong@foyer101:~$ conda env list
# conda environments:
#
                                /att/nobackup/ssstrong/conda/envs/SAvEdasStratusYMLTest
                                /att/nobackup/ssstrong/conda/envs/edas-stratus
base * /att/opt/other/centos/anaconda3
celery /att/opt/other/centos/anaconda3/envs/celery
earthml /att/opt/other/centos/anaconda3/envs/earthml
myMongo /att/opt/other/centos/anaconda3/envs/myMongo
mypsgres /att/opt/other/centos/anaconda3/envs/mypsgres
r-environment /att/opt/other/centos/anaconda3/envs/r-environment
baseclone /home/ssstrong/.conda/envs/baseclone

|ssstrong@foyer101:~$ conda activate
(base) ssstrong@foyer101:~$
```

"conda activate"
will activate the "base" conda env





Conda deactivate

```
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
                                /att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest
                                /att/nobackup/sstrong/conda/envs/edas-stratus
base                             * /att/opt/other/centos/anaconda3
celery                           /att/opt/other/centos/anaconda3/envs/celery
earthml                          /att/opt/other/centos/anaconda3/envs/earthml
myMongo                          /att/opt/other/centos/anaconda3/envs/myMongo
mypsgres                         /att/opt/other/centos/anaconda3/envs/mypsgres
r-environment                    /att/opt/other/centos/anaconda3/envs/r-environment
baseclone                        /home/sstrong/.conda/envs/baseclone

sstrong@foyer101:~$ conda activate
(base) sstrong@foyer101:~$ conda deactivate
sstrong@foyer101:~$ █
```





Conda activate another env (celery)

```
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
                                /att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest
                                /att/nobackup/sstrong/conda/envs/edas-stratus
base                             * /att/opt/other/centos/anaconda3
celery                           /att/opt/other/centos/anaconda3/envs/celery
earthml                          /att/opt/other/centos/anaconda3/envs/earthml
myMongo                          /att/opt/other/centos/anaconda3/envs/myMongo
mypsgres                         /att/opt/other/centos/anaconda3/envs/mypsgres
r-environment                    /att/opt/other/centos/anaconda3/envs/r-environment
baseclone                        /home/sstrong/.conda/envs/baseclone

sstrong@foyer101:~$ conda activate
(base) sstrong@foyer101:~$ conda deactivate
sstrong@foyer101:~$ conda activate celery
(celery) sstrong@foyer101:~$
```





Creating new conda Envs



Work on
nobackup



Create a new
env (.../envs)



Customize
and configure



Work on ../nobackup

Due to limited storage on /home/<username>, it preferred that all new conda environments be created on /att/nobackup/<username>

To accomplish this:

```
sstrong@foyer101:~$ mv ~/.conda $NOBACKUP/
```

Make a softlink:

```
sstrong@foyer101:~$ ln -s $NOBACKUP/.conda ~/.conda
```

```
sstrong@foyer101:~$ ls -alt .conda
```

```
lrwxrwxrwx 1 sstrong k3000 28 Nov  8 15:58 .conda -> /att/nobackup/sstrong/.conda
```





Create new env

```
sstrong@foyer101:~$ conda create -n SAvCondaEnv
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /home/sstrong/.conda/envs/SAvCondaEnv

Proceed ([y]/n)? y

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate SAvCondaEnv
#
# To deactivate an active environment, use
#
#     $ conda deactivate

sstrong@foyer101:~$ ls -alt /att/nobackup/sstrong/.conda
total 48
-rw-r--r--  1 sstrong k3000   178 Nov 19 17:46 environments.txt
drwxrwsr-x  4 sstrong k3000  4096 Nov 19 17:46 envs
drwxrwsr-x 66 sstrong k3000 16384 Nov 14 18:34 pkgs
drwxrwsr-x  4 sstrong k3000  4096 Nov 14 15:45 .
drwxrwxr-x  8 sstrong 40010  4096 Sep 12 15:54 ..
sstrong@foyer101:~$ ls -alt /att/nobackup/sstrong/.conda/envs
total 0
drwxrwsr-x  3 sstrong k3000 4096 Nov 19 17:46 SAvCondaEnv <-----
drwxrwsr-x  4 sstrong k3000 4096 Nov 19 17:46 .
drwxrwsr-x 23 sstrong k3000 4096 Nov 14 18:34 earthmlPlus3
drwxrwsr-x  4 sstrong k3000 4096 Nov 14 15:45 ..
-rw-r--r--  1 sstrong k3000    0 Sep 12 16:01 .conda_envs_dir_test
sstrong@foyer101:~$
```

**SAvCondaEnv is created under
/att/nobackup/sstrong/.conda/envs**





Customize and Configure

Once you have created a conda env, you can fully customize and configure your conda env by installing packages

First activate the environment..

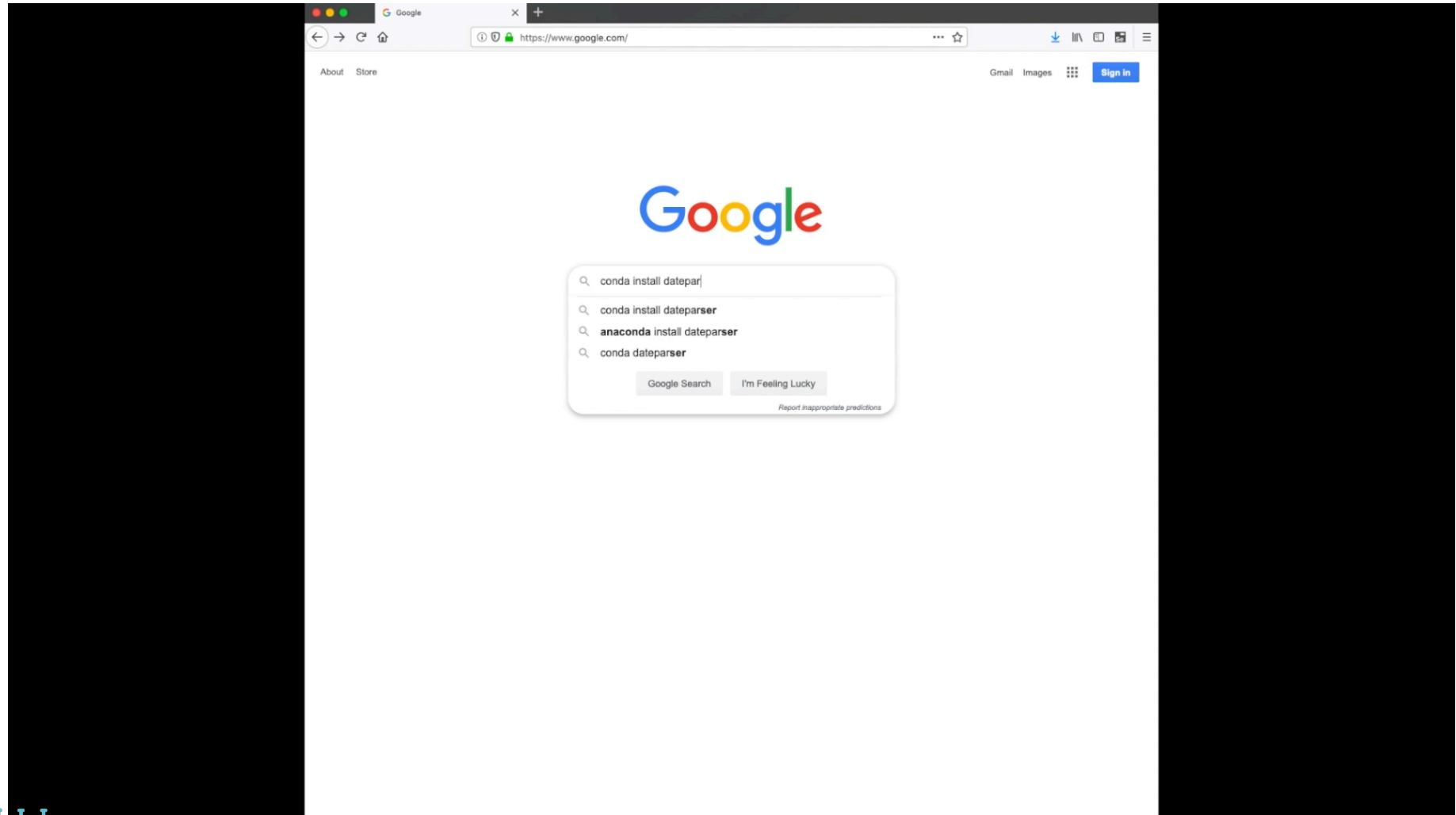
```
sstrong@foyer101:~$ conda activate SAvCondaEnv  
-----> (SAvCondaEnv) sstrong@foyer101:~$
```





Customize and Configure

In this example we will install two packages into SAvCondaEnv, dateparser and python-graphviz.
First we have to locate the conda channel for the specified package





Customize and Configure

Another option for users is to leverage a managed conda env

If a conda env exists with most the desired packages, users can copy that managed conda env by cloning it and adding additional packages.

Here we'll choose earthml to clone

```
sstrong@foyer101:~$ which conda
/att/opt/other/centos/anaconda3/condabin/conda
sstrong@foyer101:~$ conda env list
# conda environments:
#
                                /att/nobackup/sstrong/conda/envs/SAvEdasStratusYMLTest
                                /att/nobackup/sstrong/conda/envs/edas-stratus
base                             * /att/opt/other/centos/anaconda3
celery                           /att/opt/other/centos/anaconda3/envs/celery
-----> earthml                  /att/opt/other/centos/anaconda3/envs/earthml
myMongo                         /att/opt/other/centos/anaconda3/envs/myMongo
mypsgres                        /att/opt/other/centos/anaconda3/envs/mypsgres
r-environment                   /att/opt/other/centos/anaconda3/envs/r-environment
baseclone                       /home/sstrong/.conda/envs/baseclone
```





Customize and Configure

```
sstrong@foyer101:/att/nobackup/sstrong/.conda/envs$ conda create -n earthmlPlus3 --clone earthml
Source:          /att/opt/other/centos/anaconda3/envs/earthml
Destination:    /home/sstrong/.conda/envs/earthmlPlus3
Packages: 272
Files: 38
Preparing transaction: done
Verifying transaction: done
Executing transaction: - b'Enabling notebook extension jupyter-js-widgets/extension...\n      32mOK\x1b[0m\n' - Validating:
done
#
# To activate this environment, use
#
#     $ conda activate earthmlPlus3
#
# To deactivate an active environment, use
#
#     $ conda deactivate

sstrong@foyer101:/att/nobackup/sstrong/.conda/envs$ ls -alt
total 0
drwxrwsr-x 22 sstrong k3000 4096 Nov 14 16:20 earthmlPlus3 <-----
drwxrwsr-x  3 sstrong k3000 4096 Nov 14 16:20 .
drwxrwsr-x  4 sstrong k3000 4096 Nov 14 15:45 ..
-rw-r--r--  1 sstrong k3000    0 Sep 12 16:01 .conda_envs_dir_test
sstrong@foyer101:/att/nobackup/sstrong/.conda/envs$ █
```

earthmlPlus3 created with earthml env and ready
for package installation



Summary

- No Anaconda installation necessary
- Many available modules and can simply load the one you want.
- Can create new environments or leverage existing environments.



Assistance

“Anaconda on ADAPT”

instructional video located at:

<https://www.nccs.nasa.gov/nccs-users/instructional/instructional-videos>

Email:

support@nccs.nasa.gov